Piperazine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 47.0 °C

Global applicability domain: Inside

Local applicability domain index: 5.41e-01

Confidence level: 5.15e-01

Nearest Neighbors from the Training Set

Image not found
2-Methylpiperazine
Measured: 62.0
Predicted: 68.0

Image not found
2,5-Dimethylpyrazine
Measured: 15.0
Predicted: 28.8

Image not found
2,6-Dimethylpyrazine
Measured: 47.5
Predicted: 28.8

Image not found
2-Methylpyrazine
Measured: -29.0
Predicted: 35.6